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Grain-Scale Simulation of Transformation and Switching in PZT Ceramic, J.B. AIDUN, R.M. BRANNON, J. ROBBINS, Sandia National Laboratories¹ - A grain-scale simulation of the shock response of PZT ceramic is being developed to relate ceramic microstructure to its ferroelectric performance when used as the active element in a shock-actuated power supply. The aim is to apply this simulation capability to guide selection of manufacturing process steps for PZT ceramic and guide enhancements to a macroscale, homogeneous ceramic material model. To augment the numerical description of the stress-induced phase transformation in single crystal PZT,² an internal state variable model for electro-mechanically driven ferroelectric (FE) domain switching³ has been implemented in the massively parallel ALE code ALEGRA. A domain switching model is needed to validate the simulations against quasistatic test measurements and is likely to affect axial mode shock response where high electric fields are produced. The capabilities and limitations of the domain switching model will be described. Illustrative results from direct numerical simulation of the response of an aggregate of PZT grains will be given for both quasistatic and axial mode shock wave loading. The performance of the domain switching model and the importance of domain switching in PZT in the power supply application will be discussed.

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² S.T. Montgomery, p.179 in "Shock Waves in Condensed Matter," Y.M. Gupta, Ed. Plenum (New York, 1986).

³ J.E. Huber, N.A. Fleck, C.M. Landis, R.M. McMeeking, J.Mech.Phys.Solids 47, 1663 (1999).